

2-Aminopurine: A Probe of Structural Dynamics and Charge Transfer in DNA and DNA:RNA Hybrids

Melanie A. O'Neill and Jacqueline K. Barton

Division of Chemistry and Chemical Engineering

California Institute of Technology,

Pasadena, California 91125

Supporting Information

Figure S-1. Representative melting curves of 100 μM Ap-containing DNA and DNA:RNA duplexes: (a) $\text{ApA}_0\text{G-2}$; (b) $\text{apa}_0\text{g-2}$; (c) $\text{ApA}_0\text{I-2}$; (d) $\text{ApA}_0\text{I-1}$; (e) $\text{ApA}_0\text{Z-1}$; (f) $\text{apa}_0\text{z-2}$.

Figure S-2. CD spectra of DNA duplexes (closed circles) and DNA:RNA hybrids (open circles) of Type-1 ($\text{ApA}_0\text{Z-1}$ and $\text{apa}_0\text{z-1}$). The spectra were obtained at 10 $^\circ\text{C}$ using 2.5 μM duplexes in 100 mM sodium phosphate buffer pH

Figure S-3. CD spectra of I (closed circles) and G or Z (open circles) containing duplexes of (a) Type-2 DNA (ApI and ApG) and (b) Type-1 DNA:RNA (apa_3i and apa_3z). The spectra were obtained at 10 $^\circ\text{C}$ using 2.5 μM duplexes in 100 mM sodium phosphate buffer pH 7.

Figure S-4. Representative CD spectra of 2.5 μM ApI or api (closed circles) and ApA_3I or apa_3i (open circles) DNA or DNA:RNA duplexes, respectively: (a) ApI-1 and $\text{ApA}_3\text{I-1}$; (b) api-1 and $\text{apa}_3\text{i-1}$; (c) ApI-2 and $\text{ApA}_3\text{I-2}$; (d) api-2 and $\text{apa}_3\text{i-2}$.

Table S-1. Representative yields, expected, and determined (MALDI) molecular masses for single strand DNA oligonucleotides. The yields and mass determinations were made on oligonucleotides twice purified by HPLC.

Oligonucleotide	Purified Yield (μ mole)	Expected Mass (g/mole)	MALDI Mass (g/mole)
ApA ₀ C	0.43	4768	4766
ApA ₁ C	0.37	4792	4793
ApA ₂ C	0.41	4801	4798
ApA ₃ C	0.42	4801	4805
IT ₁	0.39	4888	4887
IT ₂	0.40	4878	4877
IT ₃	0.42	4869	4868
IT ₄	0.39	4869	4868
GT ₁	0.37	4903	4913
GT ₂	0.40	4893	4893
GT ₃	0.42	4884	4884
GT ₄	0.39	4884	4884

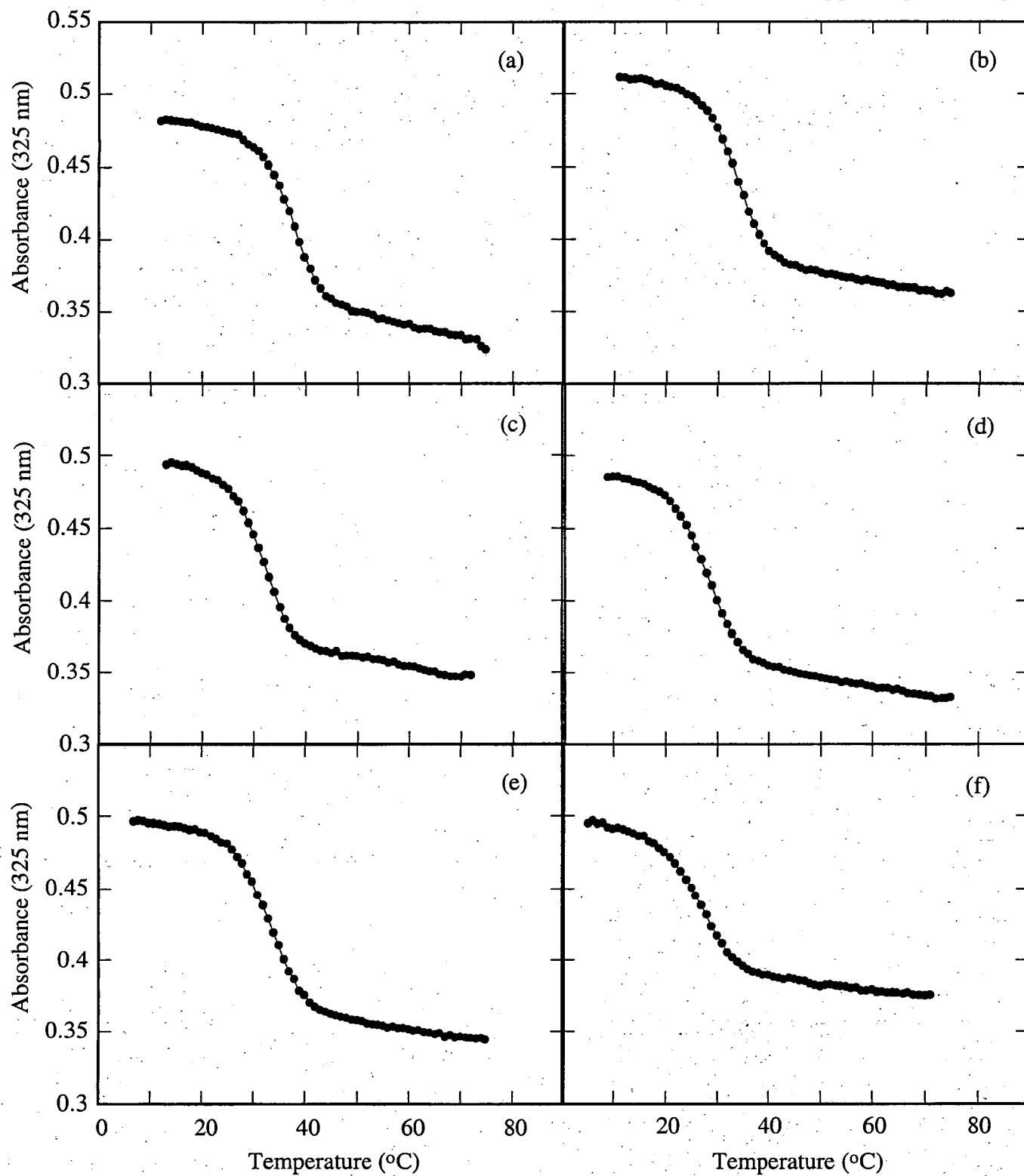


Figure S-1.

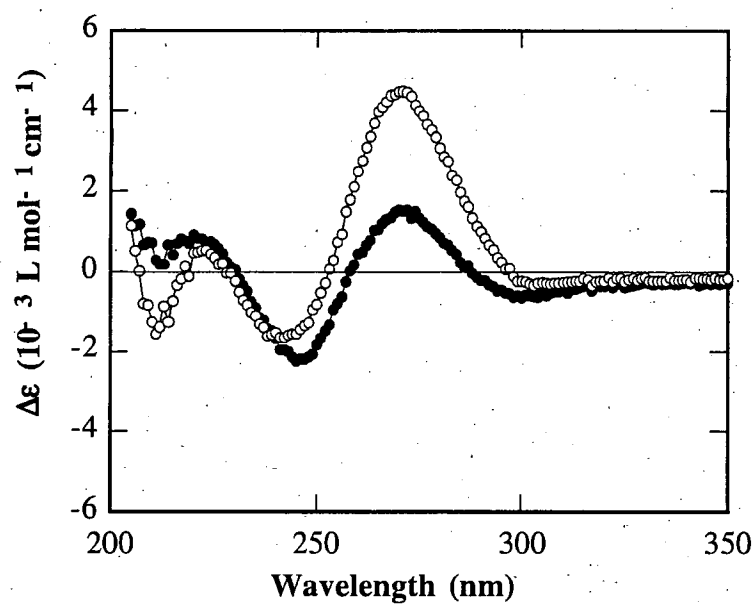


Figure S-2

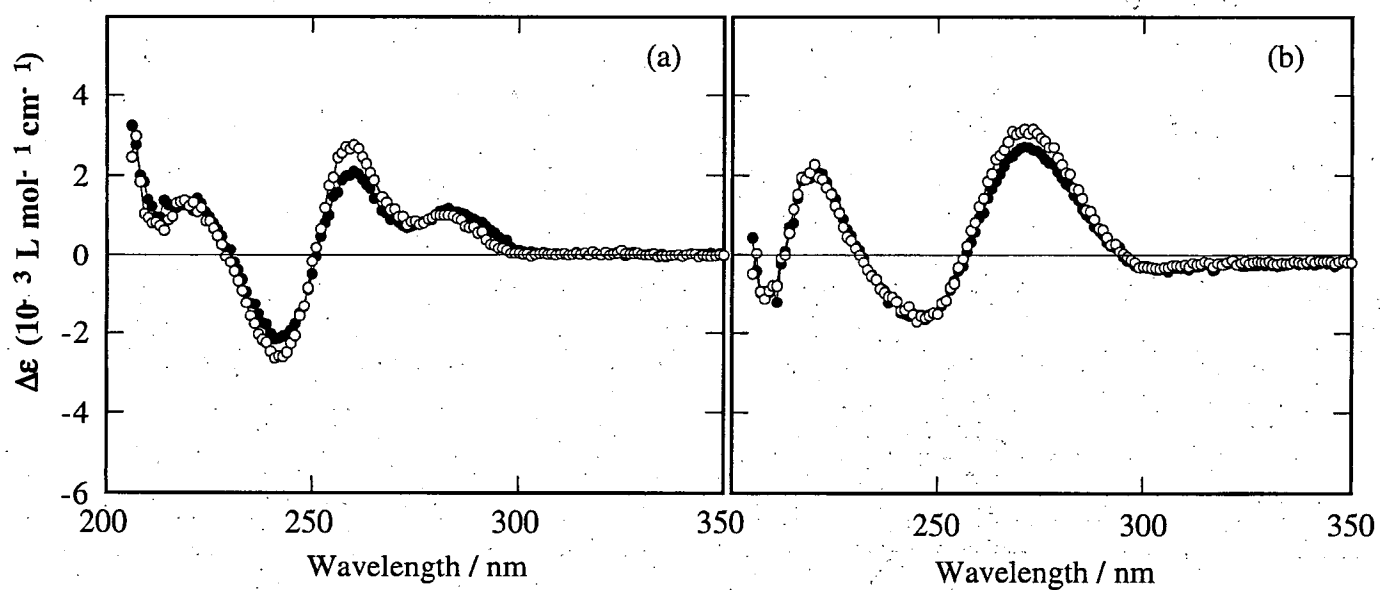


Figure S-3

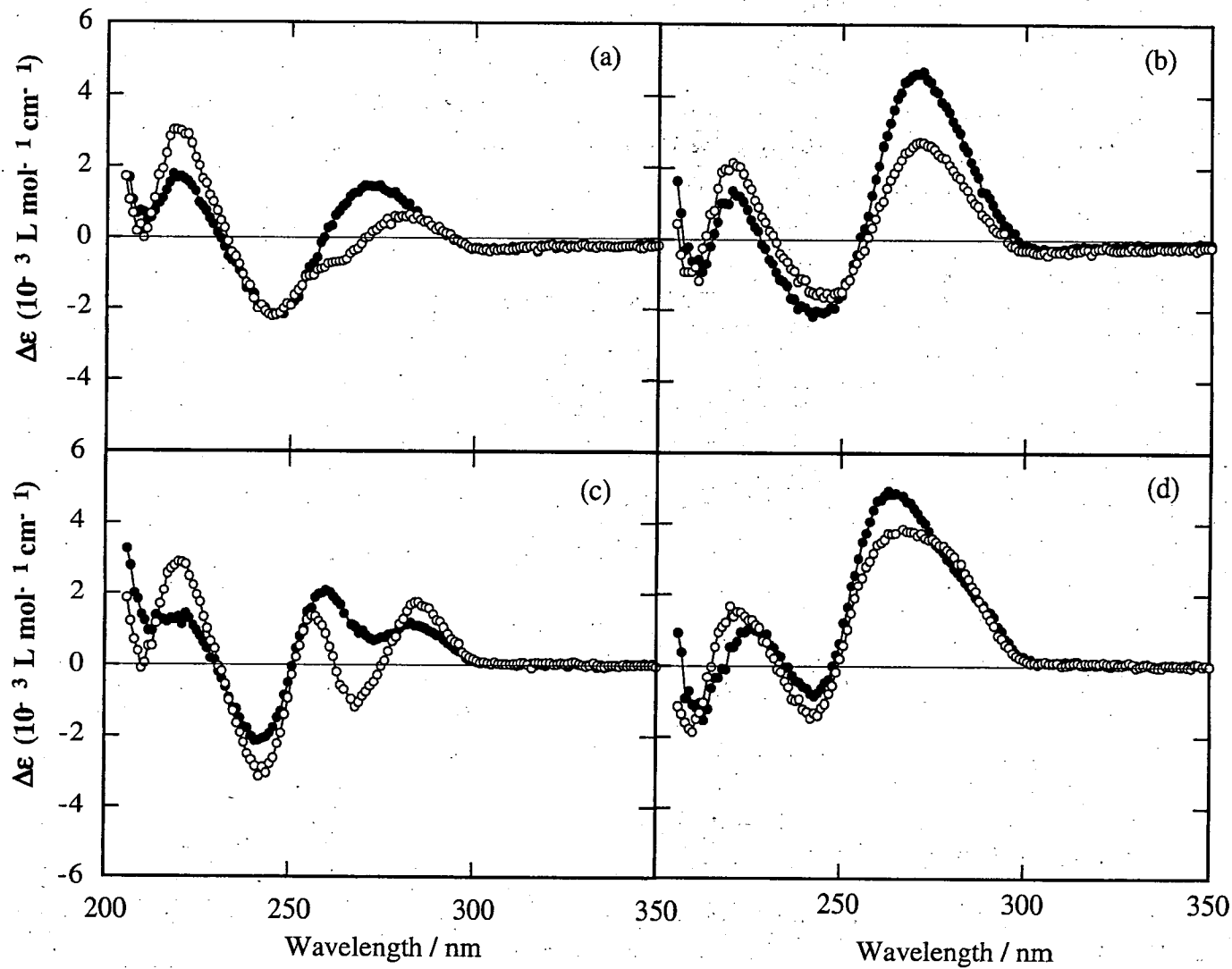


Figure S-4